



## Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 11:56 PM EDT

PDB ID : 5T4Q  
EMDB ID : EMD-8359  
Title : Autoinhibited E. coli ATP synthase state 3  
Authors : Sobti, M.; Smits, C.; Wong, A.S.W.; Ishmukhametov, R.; Stock, D.; Sandin, S.; Stewart, A.G.  
Deposited on : 2016-08-29  
Resolution : 8.53 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

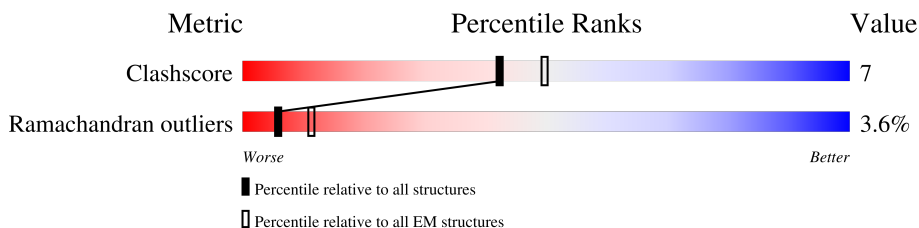
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*










The reported resolution of this entry is 8.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	 88% 12%
1	B	513	 90% 10%
1	C	513	 88% 11%
2	D	471	 87% 12%
2	E	471	 15% 86% 13%
2	F	471	 5% 86% 13%
3	G	287	 5% 85% 13%
4	H	139	 9% 85% 13%
5	I	155	 11% 92% 8%

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Mol	Chain	Length	Quality of chain
5	J	155	
6	K	271	
7	L	177	
8	M	79	
8	N	79	
8	O	79	
8	P	79	
8	Q	79	
8	R	79	
8	S	79	
8	T	79	
8	U	79	
8	V	79	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23568 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	511	Total	C	N	O	0	0
			2507	1485	511	511		
1	B	510	Total	C	N	O	0	0
			2502	1482	510	510		
1	C	508	Total	C	N	O	0	0
			2492	1476	508	508		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP B7MGF4
A	90	ALA	CYS	conflict	UNP B7MGF4
A	193	ALA	CYS	conflict	UNP B7MGF4
A	243	ALA	CYS	conflict	UNP B7MGF4
A	419	ASN	LYS	conflict	UNP B7MGF4
B	47	ALA	CYS	conflict	UNP B7MGF4
B	90	ALA	CYS	conflict	UNP B7MGF4
B	193	ALA	CYS	conflict	UNP B7MGF4
B	243	ALA	CYS	conflict	UNP B7MGF4
B	419	ASN	LYS	conflict	UNP B7MGF4
C	47	ALA	CYS	conflict	UNP B7MGF4
C	90	ALA	CYS	conflict	UNP B7MGF4
C	193	ALA	CYS	conflict	UNP B7MGF4
C	243	ALA	CYS	conflict	UNP B7MGF4
C	419	ASN	LYS	conflict	UNP B7MGF4

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	466	Total	C	N	O	0	0
			2284	1352	466	466		
2	E	466	Total	C	N	O	0	0
			2284	1352	466	466		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	466	Total 2284	C 1352	N 466	O 466	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP B7MGF2
D	-10	ARG	-	expression tag	UNP B7MGF2
D	-9	GLY	-	expression tag	UNP B7MGF2
D	-8	SER	-	expression tag	UNP B7MGF2
D	-7	HIS	-	expression tag	UNP B7MGF2
D	-6	HIS	-	expression tag	UNP B7MGF2
D	-5	HIS	-	expression tag	UNP B7MGF2
D	-4	HIS	-	expression tag	UNP B7MGF2
D	-3	HIS	-	expression tag	UNP B7MGF2
D	-2	HIS	-	expression tag	UNP B7MGF2
D	-1	GLY	-	expression tag	UNP B7MGF2
D	137	ALA	CYS	conflict	UNP B7MGF2
E	-11	MET	-	expression tag	UNP B7MGF2
E	-10	ARG	-	expression tag	UNP B7MGF2
E	-9	GLY	-	expression tag	UNP B7MGF2
E	-8	SER	-	expression tag	UNP B7MGF2
E	-7	HIS	-	expression tag	UNP B7MGF2
E	-6	HIS	-	expression tag	UNP B7MGF2
E	-5	HIS	-	expression tag	UNP B7MGF2
E	-4	HIS	-	expression tag	UNP B7MGF2
E	-3	HIS	-	expression tag	UNP B7MGF2
E	-2	HIS	-	expression tag	UNP B7MGF2
E	-1	GLY	-	expression tag	UNP B7MGF2
E	137	ALA	CYS	conflict	UNP B7MGF2
F	-11	MET	-	expression tag	UNP B7MGF2
F	-10	ARG	-	expression tag	UNP B7MGF2
F	-9	GLY	-	expression tag	UNP B7MGF2
F	-8	SER	-	expression tag	UNP B7MGF2
F	-7	HIS	-	expression tag	UNP B7MGF2
F	-6	HIS	-	expression tag	UNP B7MGF2
F	-5	HIS	-	expression tag	UNP B7MGF2
F	-4	HIS	-	expression tag	UNP B7MGF2
F	-3	HIS	-	expression tag	UNP B7MGF2
F	-2	HIS	-	expression tag	UNP B7MGF2
F	-1	GLY	-	expression tag	UNP B7MGF2
F	137	ALA	CYS	conflict	UNP B7MGF2

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	284	Total	C	N	O	0	0
			1400	832	284	284		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ASP	GLU	conflict	UNP B7MGF3
G	87	ALA	CYS	conflict	UNP B7MGF3
G	112	ALA	CYS	conflict	UNP B7MGF3

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	136	Total	C	N	O	0	0
			668	396	136	136		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	155	Total	C	N	O	0	0
			772	462	155	155		
5	J	155	Total	C	N	O	0	0
			772	462	155	155		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ALA	CYS	conflict	UNP P0ABA2
J	21	ALA	CYS	conflict	UNP P0ABA2

- Molecule 6 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	211	Total	C	N	O	0	0
			1040	618	211	211		

- Molecule 7 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	160	Total	C	N	O	0	0
			793	473	160	160		

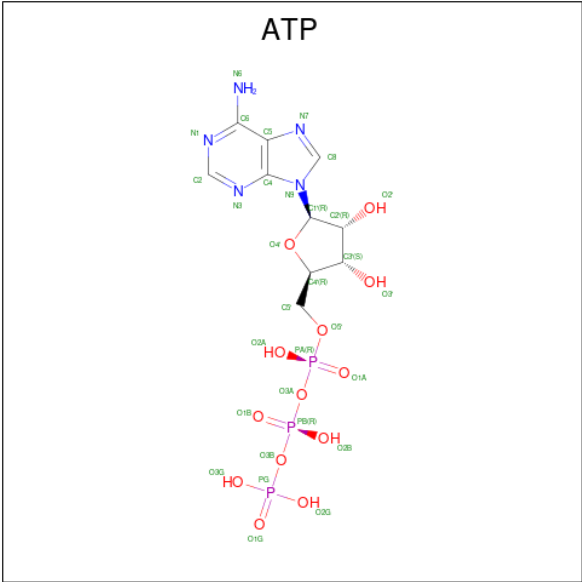
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	64	ALA	CYS	conflict	UNP B7MGF5
L	140	ALA	CYS	conflict	UNP B7MGF5

- Molecule 8 is a protein called ATP synthase subunit c.

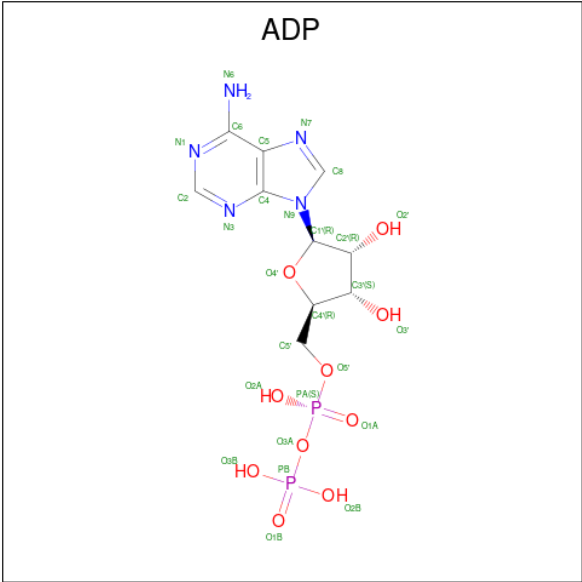
Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	75	Total	C	N	O	0	0
			365	215	75	75		
8	N	75	Total	C	N	O	0	0
			365	215	75	75		
8	O	75	Total	C	N	O	0	0
			365	215	75	75		
8	P	75	Total	C	N	O	0	0
			365	215	75	75		
8	Q	75	Total	C	N	O	0	0
			365	215	75	75		
8	R	75	Total	C	N	O	0	0
			365	215	75	75		
8	S	75	Total	C	N	O	0	0
			365	215	75	75		
8	T	75	Total	C	N	O	0	0
			365	215	75	75		
8	U	75	Total	C	N	O	0	0
			365	215	75	75		
8	V	75	Total	C	N	O	0	0
			365	215	75	75		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



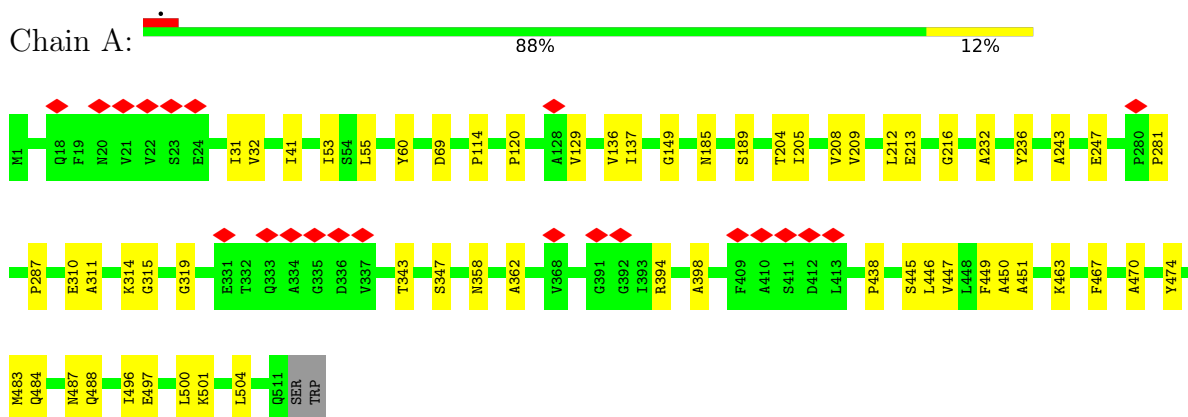


Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

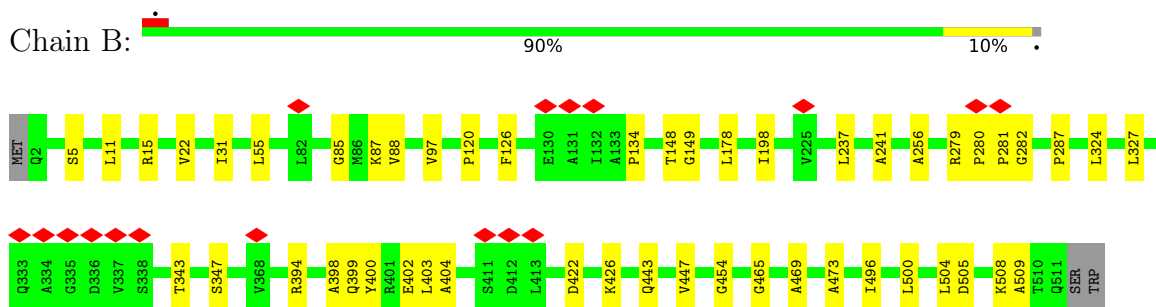
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

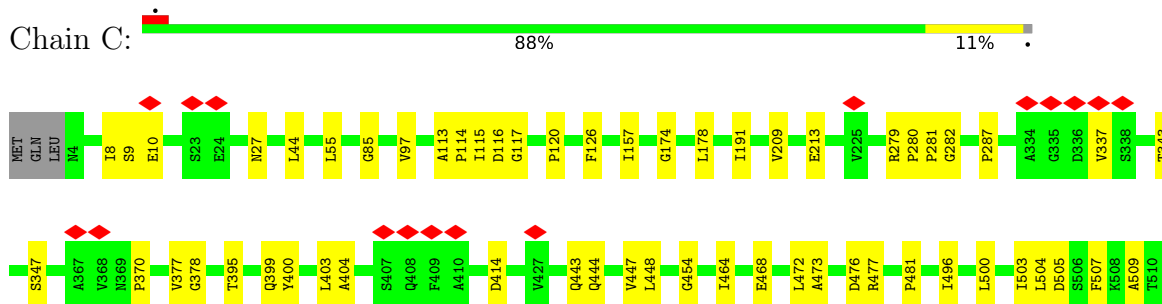
- Molecule 1: ATP synthase subunit alpha



- Molecule 1: ATP synthase subunit alpha




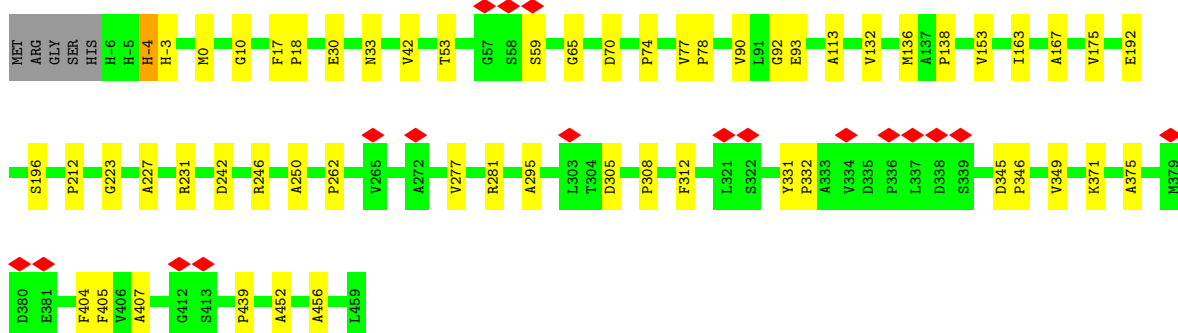
- Molecule 1: ATP synthase subunit alpha






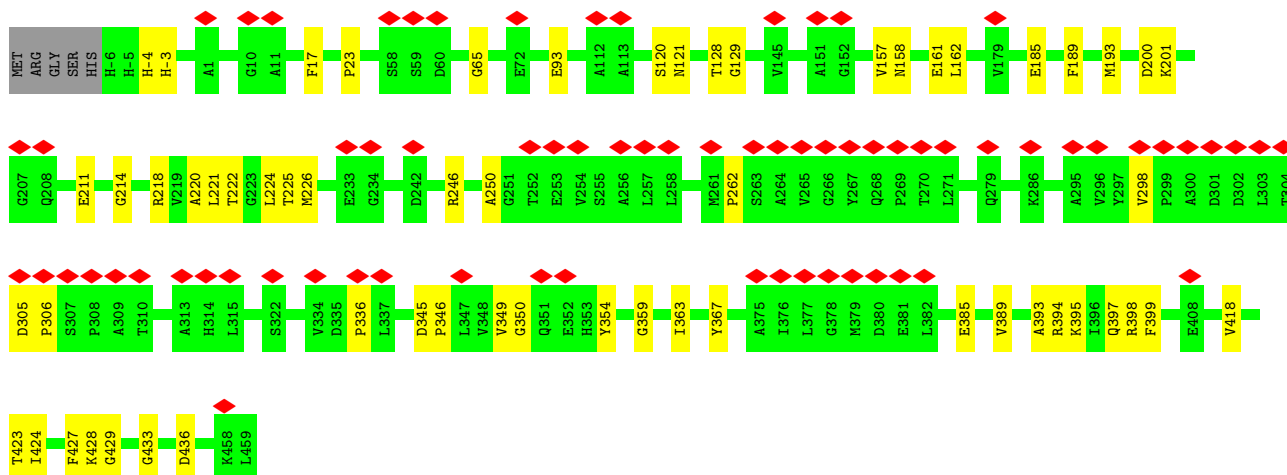
• Molecule 2: ATP synthase subunit beta

Chain D:  87% 12%




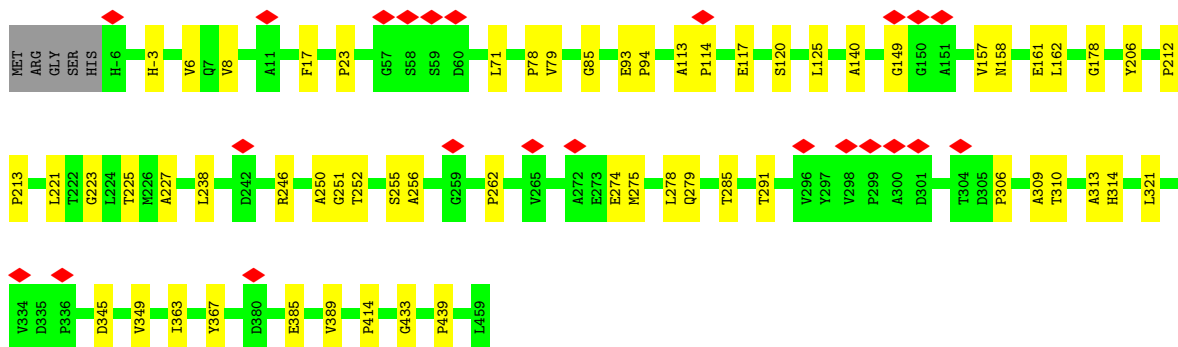
• Molecule 2: ATP synthase subunit beta

Chain E:  15% 86% 13%

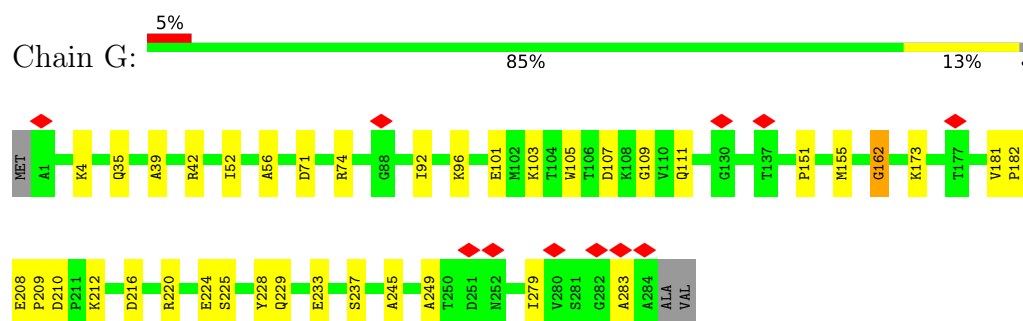


• Molecule 2: ATP synthase subunit beta

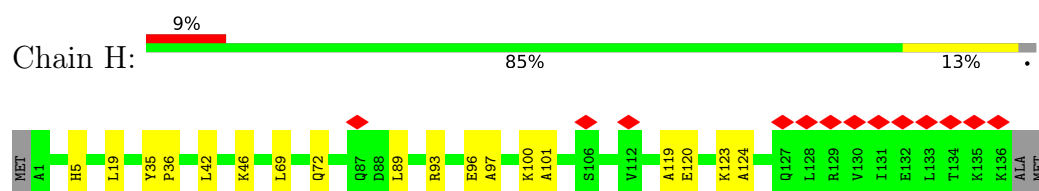
Chain F:  5% 86% 13%



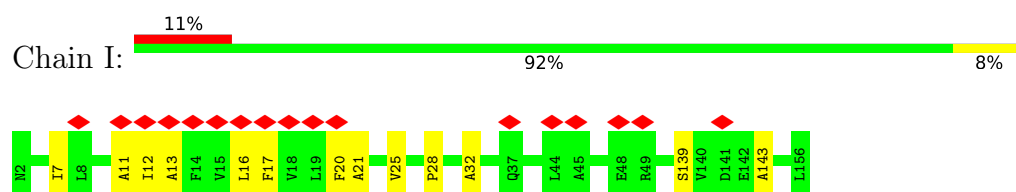
- Molecule 3: ATP synthase gamma chain



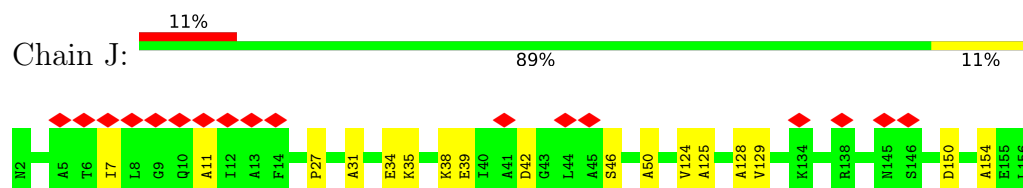
- Molecule 4: ATP synthase epsilon chain



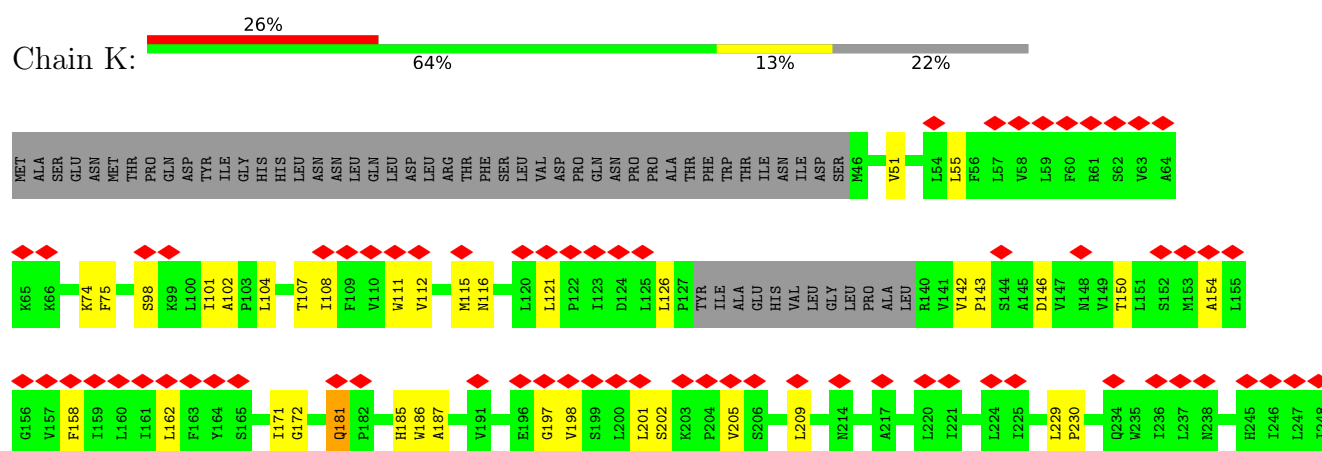
- Molecule 5: ATP synthase subunit b



- Molecule 5: ATP synthase subunit b




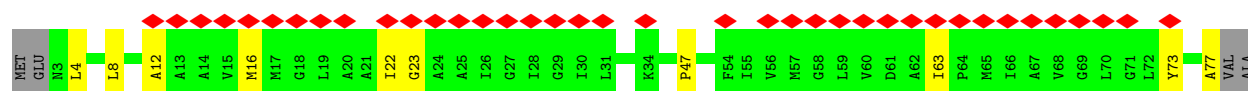
- Molecule 6: ATP synthase subunit a






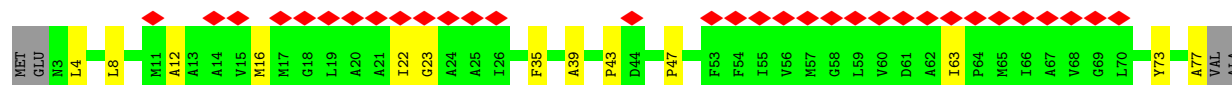
- Molecule 8: ATP synthase subunit c

Chain Q: 




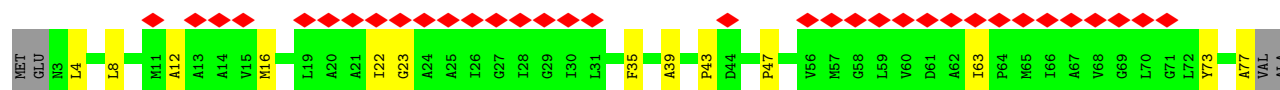
- Molecule 8: ATP synthase subunit c

Chain R: 




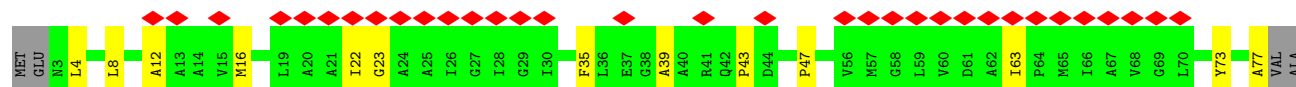
- Molecule 8: ATP synthase subunit c

Chain S: 




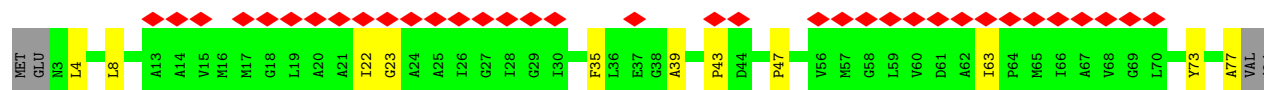
- Molecule 8: ATP synthase subunit c

Chain T: 




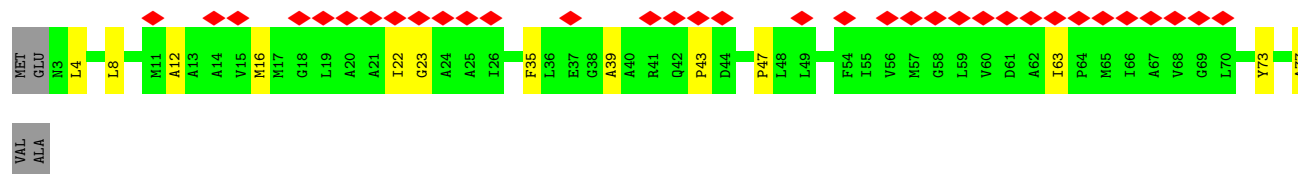
- Molecule 8: ATP synthase subunit c

Chain U: 



- Molecule 8: ATP synthase subunit c

Chain V: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95345	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	29	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.026	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	350.0, 350.0, 350.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/2506	0.43	0/3478
1	B	0.25	0/2501	0.43	0/3471
1	C	0.24	0/2491	0.43	0/3457
2	D	0.24	0/2283	0.42	0/3167
2	E	0.24	0/2283	0.43	0/3167
2	F	0.25	0/2283	0.45	0/3167
3	G	0.23	0/1399	0.39	0/1945
4	H	0.27	0/667	0.45	0/925
5	I	0.23	0/771	0.33	0/1076
5	J	0.23	0/771	0.34	0/1076
6	K	0.23	0/1038	0.41	0/1441
7	L	0.23	0/792	0.39	0/1103
8	M	0.23	0/364	0.34	0/502
8	N	0.24	0/364	0.34	0/502
8	O	0.23	0/364	0.33	0/502
8	P	0.23	0/364	0.34	0/502
8	Q	0.24	0/364	0.34	0/502
8	R	0.23	0/364	0.34	0/502
8	S	0.24	0/364	0.34	0/502
8	T	0.23	0/364	0.34	0/502
8	U	0.24	0/364	0.34	0/502
8	V	0.23	0/364	0.34	0/502
All	All	0.24	0/23425	0.41	0/32493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	1240	23	0
1	B	2502	0	1235	20	0
1	C	2492	0	1231	20	0
2	D	2284	0	1065	16	0
2	E	2284	0	1065	24	0
2	F	2284	0	1065	23	0
3	G	1400	0	665	17	0
4	H	668	0	330	8	0
5	I	772	0	406	9	0
5	J	772	0	406	11	0
6	K	1040	0	464	18	0
7	L	793	0	407	17	0
8	M	365	0	192	7	0
8	N	365	0	192	5	0
8	O	365	0	192	3	0
8	P	365	0	192	3	0
8	Q	365	0	192	5	0
8	R	365	0	192	6	0
8	S	365	0	192	6	0
8	T	365	0	192	7	0
8	U	365	0	192	5	0
8	V	365	0	192	7	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0
10	D	27	0	12	0	0
All	All	23568	0	11547	251	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:128:THR:H	2:E:129:GLY:HA2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:58:GLU:O	7:L:62:ALA:HB3	1.91	0.71
1:C:97:VAL:O	1:C:126:PHE:HA	1.91	0.71
1:A:53:ILE:O	1:A:60:TYR:HA	1.91	0.71
5:J:124:VAL:O	5:J:128:ALA:HB3	1.94	0.68
5:J:27:PRO:O	5:J:31:ALA:HB3	1.92	0.68
2:F:238:LEU:HA	2:F:291:THR:O	1.94	0.67
1:B:237:LEU:O	1:B:241:ALA:HB3	1.96	0.65
6:K:186:TRP:H	6:K:187:ALA:C	2.00	0.65
1:A:446:LEU:O	1:A:450:ALA:HB3	2.00	0.62
2:F:309:ALA:O	2:F:313:ALA:HB3	2.00	0.62
2:D:371:LYS:O	2:D:375:ALA:HB3	1.99	0.61
2:F:178:GLY:O	2:F:206:TYR:HA	2.00	0.61
1:B:400:TYR:O	1:B:404:ALA:HB3	2.02	0.59
4:H:42:LEU:HA	4:H:69:LEU:O	2.03	0.58
1:A:394:ARG:O	1:A:398:ALA:HB3	2.03	0.58
5:I:139:SER:O	5:I:143:ALA:HB2	2.04	0.58
2:E:246:ARG:O	2:E:250:ALA:HB3	2.03	0.57
1:B:31:ILE:H	1:B:87:LYS:HA	1.71	0.56
7:L:9:PRO:O	7:L:13:ALA:HB3	2.07	0.55
2:E:128:THR:N	2:E:129:GLY:HA2	2.20	0.55
8:S:73:TYR:HA	8:S:77:ALA:HB3	1.90	0.54
5:J:150:ASP:O	5:J:154:ALA:HB3	2.07	0.54
8:Q:73:TYR:HA	8:Q:77:ALA:HB3	1.90	0.54
4:H:120:GLU:O	4:H:124:ALA:HB3	2.08	0.54
3:G:52:ILE:O	3:G:56:ALA:HB2	2.08	0.53
8:M:73:TYR:HA	8:M:77:ALA:HB3	1.90	0.53
8:U:73:TYR:HA	8:U:77:ALA:HB3	1.90	0.53
2:F:246:ARG:O	2:F:250:ALA:HB3	2.09	0.53
7:L:31:LEU:O	7:L:35:ALA:HB3	2.07	0.53
8:N:73:TYR:HA	8:N:77:ALA:HB3	1.90	0.53
8:V:73:TYR:HA	8:V:77:ALA:HB3	1.90	0.53
2:D:246:ARG:O	2:D:250:ALA:HB3	2.09	0.53
3:G:279:ILE:HA	3:G:283:ALA:HB3	1.90	0.52
1:B:256:ALA:O	1:B:324:LEU:HA	2.09	0.52
8:R:73:TYR:HA	8:R:77:ALA:HB3	1.90	0.52
8:O:73:TYR:HA	8:O:77:ALA:HB3	1.91	0.52
8:P:73:TYR:HA	8:P:77:ALA:HB3	1.91	0.52
1:B:97:VAL:O	1:B:126:PHE:HA	2.10	0.52
3:G:245:ALA:O	3:G:249:ALA:HB3	2.09	0.52
6:K:74:LYS:H	6:K:75:PHE:HA	1.75	0.51
1:A:447:VAL:O	1:A:451:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:23:GLY:HA3	8:Q:22:ILE:HA	1.93	0.51
4:H:97:ALA:O	4:H:101:ALA:HB3	2.11	0.51
8:T:73:TYR:HA	8:T:77:ALA:HB3	1.91	0.50
1:A:358:ASN:O	1:A:362:ALA:HB2	2.12	0.49
1:B:394:ARG:O	1:B:398:ALA:HB3	2.11	0.49
8:N:23:GLY:HA3	8:O:22:ILE:HA	1.94	0.49
4:H:5:HIS:HA	4:H:19:LEU:HA	1.95	0.49
1:B:465:GLY:O	1:B:469:ALA:HB3	2.13	0.48
8:S:23:GLY:HA3	8:T:22:ILE:HA	1.94	0.48
1:C:27:ASN:HA	1:C:44:LEU:HA	1.94	0.48
1:A:243:ALA:O	1:A:247:GLU:CB	2.62	0.48
1:C:116:ASP:HA	1:C:117:GLY:HA2	1.53	0.48
8:M:22:ILE:HA	8:V:23:GLY:HA3	1.96	0.48
1:C:400:TYR:O	1:C:404:ALA:HB3	2.13	0.47
2:E:200:ASP:HA	2:E:201:LYS:HA	1.53	0.47
8:Q:23:GLY:HA3	8:R:22:ILE:HA	1.95	0.47
2:D:-4:HIS:HA	2:D:-3:HIS:C	2.34	0.47
5:J:124:VAL:O	5:J:128:ALA:CB	2.62	0.47
7:L:42:GLN:O	7:L:46:LEU:CB	2.63	0.47
2:E:363:ILE:O	2:E:367:TYR:CB	2.63	0.47
5:J:7:ILE:O	5:J:11:ALA:HB3	2.14	0.47
7:L:96:ILE:O	7:L:100:ALA:HB3	2.15	0.47
8:U:23:GLY:HA3	8:V:22:ILE:HA	1.96	0.47
7:L:128:MET:O	7:L:132:LEU:CB	2.63	0.47
2:E:423:THR:O	2:E:427:PHE:CB	2.62	0.47
6:K:171:ILE:HA	6:K:172:GLY:HA3	1.69	0.46
2:D:163:ILE:O	2:D:167:ALA:HB3	2.16	0.46
2:F:310:THR:O	2:F:314:HIS:CB	2.64	0.46
6:K:74:LYS:N	6:K:75:PHE:HA	2.30	0.46
5:I:17:PHE:O	5:I:21:ALA:CB	2.64	0.46
5:I:28:PRO:O	5:I:32:ALA:HB3	2.16	0.46
1:A:314:LYS:HA	1:A:315:GLY:HA2	1.66	0.46
2:E:222:THR:O	2:E:226:MET:CB	2.64	0.46
5:J:38:LYS:O	5:J:42:ASP:CB	2.63	0.46
7:L:55:THR:O	7:L:59:SER:CB	2.63	0.46
6:K:111:TRP:O	6:K:115:MET:CB	2.64	0.46
2:E:424:ILE:O	2:E:428:LYS:CB	2.64	0.45
3:G:173:LYS:H	3:G:182:PRO:HA	1.81	0.45
2:D:227:ALA:O	2:D:231:ARG:CB	2.64	0.45
5:J:34:GLU:O	5:J:38:LYS:CB	2.65	0.45
5:I:16:LEU:O	5:I:20:PHE:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:O	1:B:500:LEU:CB	2.65	0.45
2:E:395:LYS:O	2:E:399:PHE:CB	2.65	0.45
2:D:452:ALA:O	2:D:456:ALA:HB3	2.16	0.45
2:E:-4:HIS:HA	2:E:-3:HIS:HA	1.49	0.45
5:I:7:ILE:O	5:I:11:ALA:HB3	2.16	0.45
1:B:469:ALA:O	1:B:473:ALA:HB3	2.17	0.44
6:K:154:ALA:O	6:K:158:PHE:CB	2.65	0.44
6:K:198:VAL:O	6:K:202:SER:CB	2.65	0.44
1:A:497:GLU:O	1:A:501:LYS:CB	2.66	0.44
2:F:125:LEU:HA	2:F:140:ALA:HA	1.99	0.44
3:G:35:GLN:O	3:G:39:ALA:CB	2.66	0.44
1:C:157:ILE:HA	1:C:378:GLY:HA2	1.99	0.44
2:E:129:GLY:HA3	2:E:418:VAL:H	1.82	0.44
2:F:221:LEU:O	2:F:225:THR:CB	2.66	0.44
2:E:359:GLY:O	2:E:363:ILE:CB	2.66	0.44
1:C:468:GLU:O	1:C:472:LEU:CB	2.66	0.44
3:G:71:ASP:H	3:G:162:GLY:HA2	1.82	0.44
8:V:12:ALA:O	8:V:16:MET:CB	2.65	0.44
3:G:101:GLU:O	3:G:105:TRP:CB	2.65	0.44
3:G:220:ARG:O	3:G:224:GLU:CB	2.66	0.44
8:R:23:GLY:HA3	8:S:22:ILE:HA	2.00	0.44
1:A:232:ALA:O	1:A:236:TYR:CB	2.66	0.44
5:J:42:ASP:O	5:J:46:SER:CB	2.66	0.44
7:L:28:GLN:O	7:L:32:ALA:HB3	2.18	0.44
2:D:42:VAL:HA	2:D:53:THR:HA	1.99	0.44
3:G:225:SER:O	3:G:229:GLN:CB	2.66	0.44
6:K:158:PHE:O	6:K:162:LEU:CB	2.66	0.44
6:K:205:VAL:O	6:K:209:LEU:CB	2.66	0.44
7:L:149:GLY:O	7:L:153:ARG:CB	2.66	0.44
2:E:189:PHE:O	2:E:193:MET:CB	2.66	0.43
8:M:12:ALA:O	8:M:16:MET:CB	2.65	0.43
8:S:4:LEU:O	8:S:8:LEU:CB	2.66	0.43
1:C:399:GLN:O	1:C:403:LEU:CB	2.66	0.43
1:C:395:THR:O	1:C:399:GLN:CB	2.67	0.43
1:C:473:ALA:O	1:C:477:ARG:CB	2.66	0.43
8:U:4:LEU:O	8:U:8:LEU:CB	2.65	0.43
1:A:445:SER:O	1:A:449:PHE:CB	2.67	0.43
2:D:242:ASP:HA	2:D:295:ALA:HB3	2.00	0.43
2:F:252:THR:O	2:F:256:ALA:HB3	2.18	0.43
2:E:221:LEU:O	2:E:225:THR:CB	2.66	0.43
8:M:23:GLY:HA3	8:N:22:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:350:GLY:O	2:E:354:TYR:CB	2.67	0.43
2:E:394:ARG:O	2:E:398:ARG:CB	2.67	0.43
2:F:223:GLY:O	2:F:227:ALA:HB3	2.18	0.43
8:M:35:PHE:O	8:M:39:ALA:CB	2.66	0.43
1:B:465:GLY:O	1:B:469:ALA:CB	2.67	0.43
1:C:496:ILE:O	1:C:500:LEU:CB	2.67	0.43
8:N:4:LEU:O	8:N:8:LEU:CB	2.66	0.43
8:V:4:LEU:O	8:V:8:LEU:CB	2.67	0.43
1:C:472:LEU:O	1:C:476:ASP:CB	2.67	0.43
2:D:308:PRO:O	2:D:312:PHE:CB	2.67	0.43
3:G:173:LYS:CB	3:G:181:VAL:O	2.67	0.43
4:H:93:ARG:O	4:H:97:ALA:HB3	2.19	0.43
1:A:343:THR:O	1:A:347:SER:CB	2.67	0.42
2:D:30:GLU:H	2:D:70:ASP:HA	1.84	0.42
3:G:224:GLU:O	3:G:228:TYR:CB	2.67	0.42
4:H:96:GLU:O	4:H:100:LYS:CB	2.67	0.42
2:E:120:SER:HA	2:E:121:ASN:HA	1.49	0.42
5:J:35:LYS:O	5:J:39:GLU:CB	2.67	0.42
8:P:4:LEU:O	8:P:8:LEU:CB	2.67	0.42
8:S:12:ALA:O	8:S:16:MET:CB	2.67	0.42
8:V:35:PHE:O	8:V:39:ALA:CB	2.67	0.42
2:D:10:GLY:HA2	2:D:59:SER:H	1.85	0.42
6:K:104:LEU:O	6:K:108:ILE:CB	2.68	0.42
7:L:59:SER:O	7:L:63:VAL:CB	2.68	0.42
1:A:208:VAL:O	1:A:212:LEU:CB	2.68	0.42
1:B:469:ALA:O	1:B:473:ALA:CB	2.67	0.42
1:C:464:ILE:O	1:C:468:GLU:CB	2.67	0.42
6:K:146:ASP:O	6:K:150:THR:CB	2.67	0.42
2:F:246:ARG:O	2:F:250:ALA:CB	2.67	0.42
1:B:505:ASP:O	1:B:509:ALA:HB3	2.19	0.42
2:F:363:ILE:O	2:F:367:TYR:CB	2.67	0.42
5:I:17:PHE:O	5:I:21:ALA:HB3	2.20	0.42
6:K:107:THR:O	6:K:111:TRP:CB	2.68	0.42
8:O:4:LEU:O	8:O:8:LEU:CB	2.68	0.42
8:S:35:PHE:O	8:S:39:ALA:CB	2.68	0.42
3:G:151:PRO:O	3:G:155:MET:CB	2.67	0.42
8:Q:12:ALA:O	8:Q:16:MET:CB	2.68	0.42
8:T:35:PHE:O	8:T:39:ALA:CB	2.67	0.42
5:I:13:ALA:O	5:I:17:PHE:CB	2.68	0.42
6:K:197:GLY:O	6:K:201:LEU:CB	2.67	0.42
8:N:35:PHE:O	8:N:39:ALA:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLN:O	1:B:403:LEU:CB	2.68	0.42
1:B:422:ASP:O	1:B:426:LYS:CB	2.68	0.42
2:D:277:VAL:O	2:D:281:ARG:CB	2.68	0.42
3:G:233:GLU:O	3:G:237:SER:CB	2.68	0.42
7:L:31:LEU:O	7:L:35:ALA:CB	2.68	0.42
7:L:94:GLN:O	7:L:98:LEU:CB	2.68	0.42
8:M:4:LEU:O	8:M:8:LEU:CB	2.68	0.42
2:F:306:PRO:O	2:F:310:THR:CB	2.68	0.42
5:I:21:ALA:O	5:I:25:VAL:CB	2.68	0.42
5:J:125:ALA:O	5:J:129:VAL:CB	2.68	0.42
7:L:32:ALA:O	7:L:36:GLU:CB	2.67	0.42
8:T:35:PHE:O	8:T:39:ALA:HB3	2.20	0.42
1:A:500:LEU:O	1:A:504:LEU:CB	2.68	0.41
6:K:181:GLN:O	6:K:185:HIS:CB	2.67	0.41
7:L:126:ALA:O	7:L:130:LYS:CB	2.68	0.41
7:L:153:ARG:O	7:L:157:MET:CB	2.68	0.41
1:B:398:ALA:O	1:B:402:GLU:CB	2.68	0.41
1:C:500:LEU:O	1:C:504:LEU:CB	2.68	0.41
1:A:204:THR:O	1:A:208:VAL:CB	2.68	0.41
1:C:209:VAL:O	1:C:213:GLU:CB	2.69	0.41
2:F:385:GLU:O	2:F:389:VAL:CB	2.69	0.41
1:C:343:THR:O	1:C:347:SER:CB	2.68	0.41
2:E:157:VAL:O	2:E:161:GLU:CB	2.68	0.41
2:E:185:GLU:O	2:E:189:PHE:CB	2.68	0.41
2:F:149:GLY:HA3	2:F:321:LEU:H	1.84	0.41
2:F:275:MET:O	2:F:279:GLN:CB	2.68	0.41
8:R:35:PHE:O	8:R:39:ALA:CB	2.69	0.41
1:B:504:LEU:O	1:B:508:LYS:CB	2.69	0.41
1:A:209:VAL:O	1:A:213:GLU:CB	2.69	0.41
1:B:343:THR:O	1:B:347:SER:CB	2.69	0.41
2:D:404:PHE:H	2:D:407:ALA:HB3	1.86	0.41
3:G:103:LYS:O	3:G:107:ASP:CB	2.69	0.41
5:J:46:SER:O	5:J:50:ALA:CB	2.69	0.41
8:T:4:LEU:O	8:T:8:LEU:CB	2.68	0.41
1:A:496:ILE:O	1:A:500:LEU:CB	2.68	0.41
1:B:11:LEU:O	1:B:15:ARG:CB	2.68	0.41
1:C:444:GLN:O	1:C:448:LEU:CB	2.68	0.41
2:D:132:VAL:O	2:D:136:MET:CB	2.68	0.41
7:L:148:ALA:O	7:L:152:ILE:CB	2.68	0.41
8:Q:4:LEU:O	8:Q:8:LEU:CB	2.69	0.41
8:R:4:LEU:O	8:R:8:LEU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:-3:HIS:HA	2:F:71:LEU:HA	2.02	0.41
6:K:51:VAL:O	6:K:55:LEU:CB	2.69	0.41
2:E:393:ALA:O	2:E:397:GLN:CB	2.68	0.41
2:F:157:VAL:O	2:F:161:GLU:CB	2.69	0.41
3:G:74:ARG:HA	3:G:111:GLN:H	1.85	0.41
8:M:35:PHE:O	8:M:39:ALA:HB3	2.20	0.41
8:V:35:PHE:O	8:V:39:ALA:HB3	2.20	0.41
1:A:185:ASN:O	1:A:189:SER:CB	2.68	0.41
1:C:8:ILE:O	1:C:10:GLU:N	2.54	0.41
2:D:192:GLU:O	2:D:196:SER:CB	2.69	0.41
2:F:274:GLU:O	2:F:278:LEU:CB	2.69	0.41
7:L:95:PHE:O	7:L:99:ARG:CB	2.69	0.41
1:A:31:ILE:HA	1:A:41:ILE:HA	2.03	0.40
1:C:503:ILE:O	1:C:507:PHE:CB	2.68	0.40
2:D:223:GLY:O	2:D:227:ALA:HB3	2.21	0.40
2:E:220:ALA:O	2:E:224:LEU:CB	2.69	0.40
2:F:251:GLY:O	2:F:255:SER:CB	2.69	0.40
4:H:97:ALA:O	4:H:101:ALA:CB	2.69	0.40
2:E:385:GLU:O	2:E:389:VAL:CB	2.69	0.40
2:F:223:GLY:O	2:F:227:ALA:CB	2.69	0.40
3:G:212:LYS:O	3:G:216:ASP:CB	2.69	0.40
6:K:150:THR:O	6:K:154:ALA:CB	2.70	0.40
8:T:23:GLY:HA3	8:U:22:ILE:HA	2.04	0.40
1:A:205:ILE:O	1:A:209:VAL:CB	2.69	0.40
1:A:463:LYS:O	1:A:467:PHE:CB	2.69	0.40
1:A:470:ALA:O	1:A:474:TYR:CB	2.69	0.40
1:A:484:GLN:O	1:A:488:GLN:CB	2.69	0.40
1:B:500:LEU:O	1:B:504:LEU:CB	2.69	0.40
2:E:158:ASN:O	2:E:162:LEU:CB	2.69	0.40
5:I:12:ILE:O	5:I:16:LEU:CB	2.69	0.40
6:K:112:VAL:O	6:K:116:ASN:CB	2.70	0.40
8:T:12:ALA:O	8:T:16:MET:CB	2.69	0.40
1:A:483:MET:O	1:A:487:ASN:CB	2.69	0.40
1:B:443:GLN:O	1:B:447:VAL:CB	2.70	0.40
1:C:505:ASP:O	1:C:509:ALA:HB2	2.21	0.40
2:F:158:ASN:O	2:F:162:LEU:CB	2.69	0.40
4:H:119:ALA:O	4:H:123:LYS:CB	2.70	0.40
6:K:108:ILE:O	6:K:112:VAL:CB	2.69	0.40
8:U:35:PHE:O	8:U:39:ALA:CB	2.70	0.40
1:C:443:GLN:O	1:C:447:VAL:CB	2.70	0.40
2:E:214:GLY:O	2:E:218:ARG:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:SER:H	2:F:285:THR:HA	1.86	0.40
2:F:309:ALA:O	2:F:313:ALA:CB	2.69	0.40
3:G:92:ILE:O	3:G:96:LYS:CB	2.69	0.40
8:R:12:ALA:O	8:R:16:MET:CB	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/513 (99%)	395 (78%)	98 (19%)	16 (3%)	4	27
1	B	508/513 (99%)	396 (78%)	94 (18%)	18 (4%)	3	25
1	C	506/513 (99%)	392 (78%)	93 (18%)	21 (4%)	3	22
2	D	464/471 (98%)	365 (79%)	73 (16%)	26 (6%)	2	19
2	E	464/471 (98%)	358 (77%)	90 (19%)	16 (3%)	3	26
2	F	464/471 (98%)	367 (79%)	77 (17%)	20 (4%)	2	22
3	G	282/287 (98%)	240 (85%)	34 (12%)	8 (3%)	5	30
4	H	134/139 (96%)	108 (81%)	21 (16%)	5 (4%)	3	24
5	I	153/155 (99%)	147 (96%)	6 (4%)	0	100	100
5	J	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
6	K	207/271 (76%)	175 (84%)	22 (11%)	10 (5%)	2	21
7	L	158/177 (89%)	130 (82%)	26 (16%)	2 (1%)	12	48
8	M	73/79 (92%)	66 (90%)	5 (7%)	2 (3%)	5	31
8	N	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	O	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	P	73/79 (92%)	65 (89%)	5 (7%)	3 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	73/79 (92%)	65 (89%)	6 (8%)	2 (3%)	5	31
8	R	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	S	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	T	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	U	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
8	V	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	23
All	All	4732/4926 (96%)	3877 (82%)	685 (14%)	170 (4%)	6	25

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	120	PRO
1	A	281	PRO
1	B	55	LEU
1	B	279	ARG
1	B	281	PRO
1	B	287	PRO
1	C	55	LEU
1	C	279	ARG
2	D	17	PHE
2	D	77	VAL
2	D	138	PRO
2	D	332	PRO
2	D	345	ASP
2	D	346	PRO
2	E	17	PHE
2	E	23	PRO
2	E	211	GLU
2	E	262	PRO
2	E	298	VAL
2	E	305	ASP
2	E	345	ASP
2	F	17	PHE
2	F	113	ALA
2	F	262	PRO
3	G	189	PRO
3	G	209	PRO
3	G	210	ASP
4	H	35	TYR

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Mol	Chain	Res	Type
4	H	72	GLN
6	K	102	ALA
6	K	126	LEU
6	K	143	PRO
6	K	181	GLN
6	K	230	PRO
8	M	47	PRO
8	M	63	ILE
8	N	47	PRO
8	N	63	ILE
8	O	47	PRO
8	O	63	ILE
8	P	47	PRO
8	P	63	ILE
8	Q	47	PRO
8	Q	63	ILE
8	R	47	PRO
8	R	63	ILE
8	S	47	PRO
8	S	63	ILE
8	T	47	PRO
8	T	63	ILE
8	U	47	PRO
8	U	63	ILE
8	V	47	PRO
8	V	63	ILE
1	A	137	ILE
1	A	438	PRO
1	C	9	SER
1	C	85	GLY
1	C	120	PRO
2	D	78	PRO
2	D	90	VAL
2	D	405	PHE
2	E	93	GLU
2	E	346	PRO
2	E	349	VAL
4	H	46	LYS
7	L	4	ILE
1	A	114	PRO
1	A	319	GLY
1	B	5	SER

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Mol	Chain	Res	Type
1	B	85	GLY
1	B	327	LEU
1	B	454	GLY
1	C	191	ILE
1	C	414	ASP
1	C	481	PRO
2	D	0	MET
2	D	74	PRO
2	E	65	GLY
2	F	79	VAL
2	F	93	GLU
2	F	117	GLU
2	F	212	PRO
2	F	414	PRO
2	F	439	PRO
3	G	4	LYS
3	G	42	ARG
3	G	162	GLY
4	H	89	LEU
6	K	142	VAL
8	O	46	ILE
1	A	69	ASP
1	A	149	GLY
1	A	310	GLU
1	A	311	ALA
1	B	88	VAL
1	B	178	LEU
1	C	114	PRO
1	C	174	GLY
1	C	178	LEU
1	C	287	PRO
2	D	18	PRO
2	D	65	GLY
2	D	93	GLU
2	D	439	PRO
2	E	336	PRO
2	E	429	GLY
2	E	436	ASP
2	F	6	VAL
2	F	94	PRO
2	F	349	VAL
3	G	208	GLU

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Mol	Chain	Res	Type
6	K	98	SER
6	K	229	LEU
1	A	216	GLY
1	A	287	PRO
1	B	22	VAL
1	B	120	PRO
1	B	134	PRO
1	B	280	PRO
1	C	280	PRO
1	C	281	PRO
2	D	305	ASP
2	D	349	VAL
2	F	23	PRO
2	F	78	PRO
2	F	85	GLY
2	F	213	PRO
2	F	345	ASP
3	G	109	GLY
8	P	46	ILE
1	A	129	VAL
1	B	148	THR
1	C	370	PRO
2	D	-4	HIS
2	D	33	ASN
2	E	306	PRO
2	E	433	GLY
1	B	149	GLY
1	C	113	ALA
2	D	331	TYR
6	K	121	LEU
1	A	136	VAL
1	C	282	GLY
2	D	262	PRO
2	F	433	GLY
4	H	36	PRO
1	B	198	ILE
1	C	377	VAL
1	C	454	GLY
2	D	113	ALA
2	D	175	VAL
2	D	212	PRO
6	K	101	ILE

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Mol	Chain	Res	Type
7	L	124	ILE
8	T	43	PRO
8	U	43	PRO
1	A	32	VAL
1	C	337	VAL
8	N	43	PRO
8	S	43	PRO
1	B	282	GLY
1	C	115	ILE
2	D	92	GLY
2	D	153	VAL
2	F	8	VAL
2	F	114	PRO
8	R	43	PRO
8	V	43	PRO

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ATP	B	601	-	26,33,33	0.93	1 (3%)	31,52,52	1.57	5 (16%)
9	ATP	A	601	-	26,33,33	0.93	1 (3%)	31,52,52	1.57	5 (16%)
9	ATP	C	601	-	26,33,33	0.94	1 (3%)	31,52,52	1.56	5 (16%)
10	ADP	D	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	B	601	-	-	1/18/38/38	0/3/3/3
9	ATP	A	601	-	-	1/18/38/38	0/3/3/3
9	ATP	C	601	-	-	1/18/38/38	0/3/3/3
10	ADP	D	601	-	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	ATP	C5-C4	2.51	1.47	1.40
9	B	601	ATP	C5-C4	2.51	1.47	1.40
9	C	601	ATP	C5-C4	2.51	1.47	1.40
10	D	601	ADP	C5-C4	2.49	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	601	ATP	PA-O3A-PB	-3.59	120.50	132.83
9	A	601	ATP	PA-O3A-PB	-3.59	120.50	132.83
9	B	601	ATP	PA-O3A-PB	-3.57	120.56	132.83
9	A	601	ATP	PB-O3B-PG	-3.49	120.84	132.83
9	C	601	ATP	PB-O3B-PG	-3.48	120.87	132.83
9	B	601	ATP	PB-O3B-PG	-3.48	120.88	132.83
9	B	601	ATP	C3'-C2'-C1'	3.27	105.91	100.98
10	D	601	ADP	C3'-C2'-C1'	3.24	105.86	100.98
9	C	601	ATP	C3'-C2'-C1'	3.24	105.86	100.98
10	D	601	ADP	PA-O3A-PB	-3.23	121.74	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	601	ATP	C3'-C2'-C1'	3.23	105.84	100.98
9	A	601	ATP	N3-C2-N1	-3.19	123.69	128.68
9	B	601	ATP	N3-C2-N1	-3.16	123.73	128.68
9	C	601	ATP	N3-C2-N1	-3.16	123.74	128.68
10	D	601	ADP	N3-C2-N1	-3.14	123.77	128.68
10	D	601	ADP	C4-C5-N7	-2.71	106.57	109.40
9	C	601	ATP	C4-C5-N7	-2.71	106.58	109.40
9	B	601	ATP	C4-C5-N7	-2.69	106.59	109.40
9	A	601	ATP	C4-C5-N7	-2.67	106.62	109.40

There are no chirality outliers.

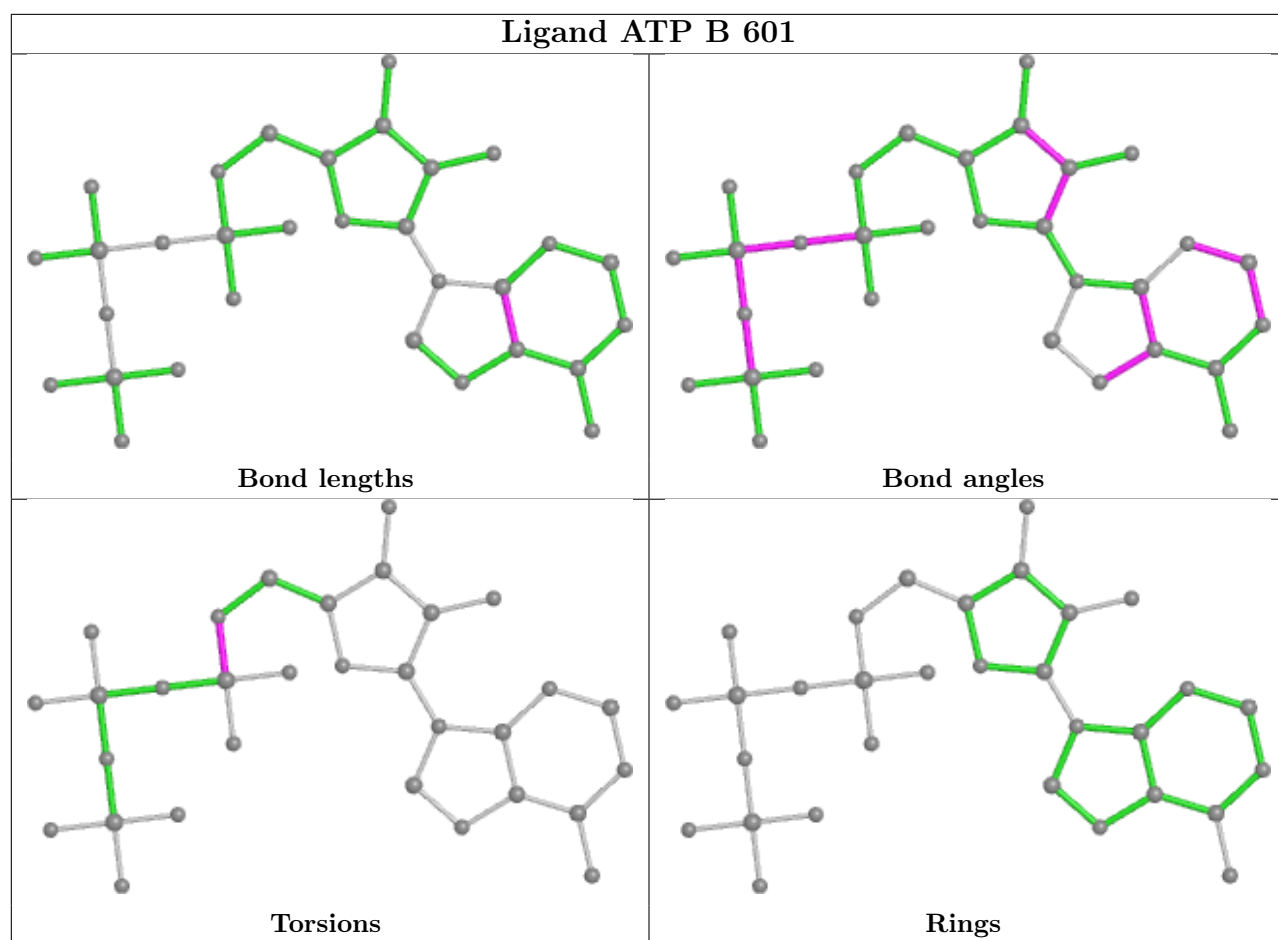
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	601	ADP	PB-O3A-PA-O1A
10	D	601	ADP	PB-O3A-PA-O2A
10	D	601	ADP	O4'-C4'-C5'-O5'
9	A	601	ATP	C5'-O5'-PA-O1A
9	B	601	ATP	C5'-O5'-PA-O1A
9	C	601	ATP	C5'-O5'-PA-O1A

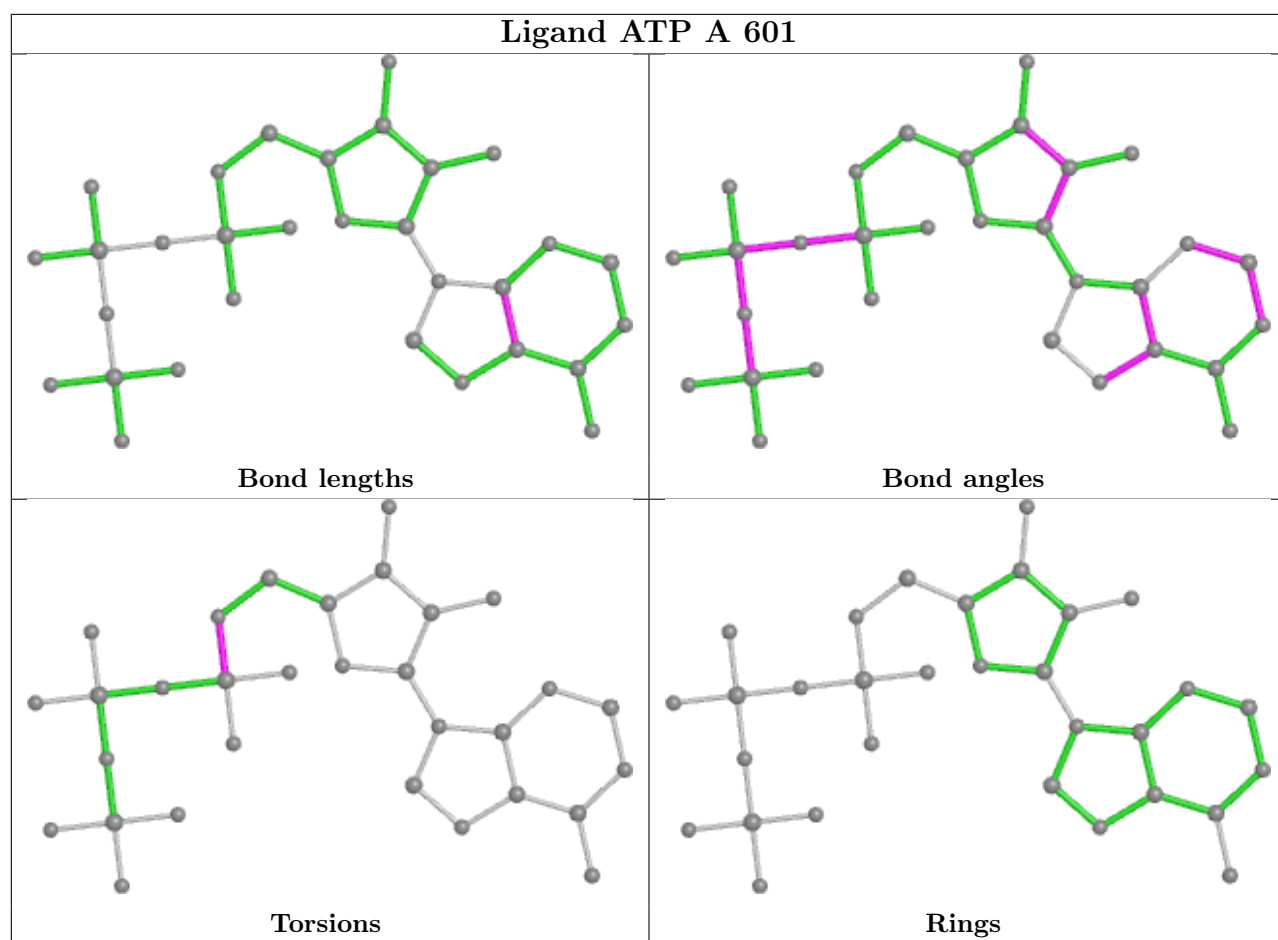
There are no ring outliers.

No monomer is involved in short contacts.

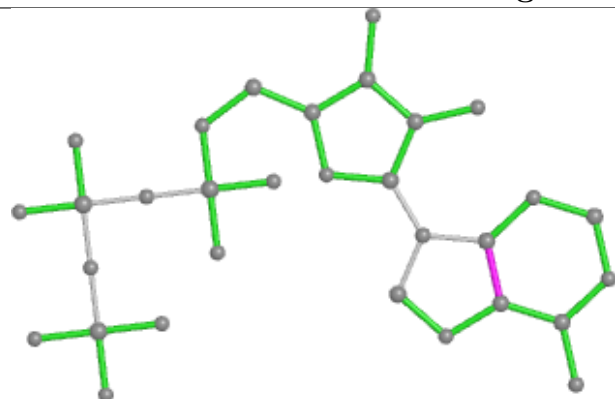
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



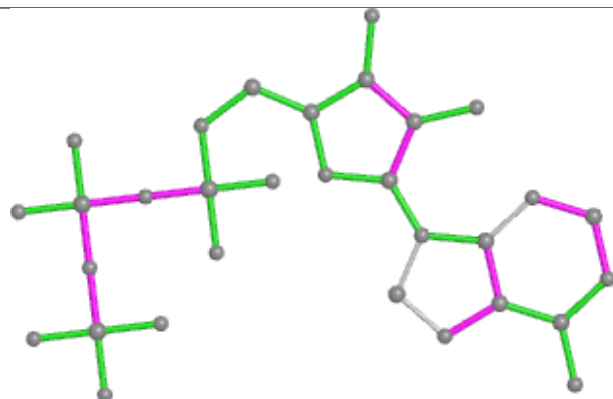




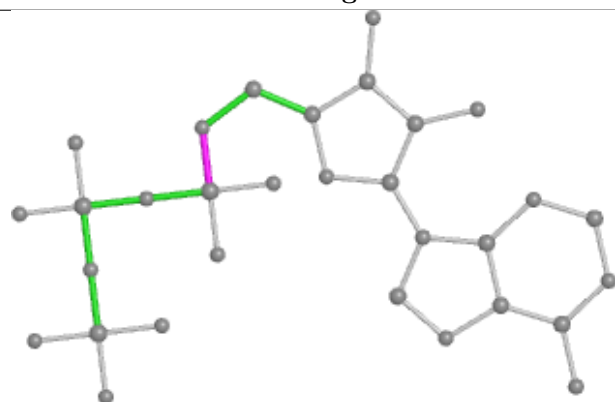
## Ligand ATP C 601



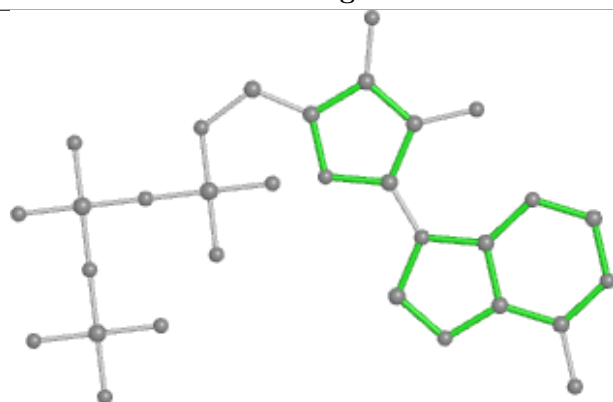
Bond lengths



Bond angles

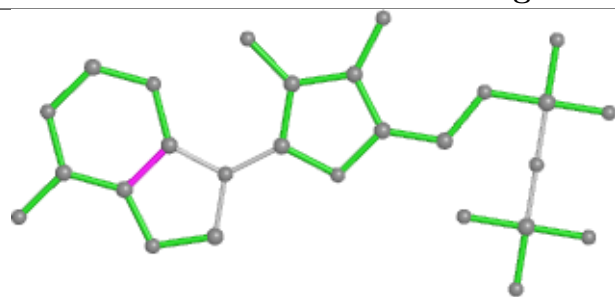


Torsions

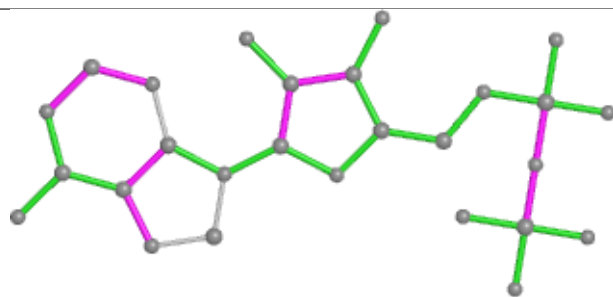


Rings

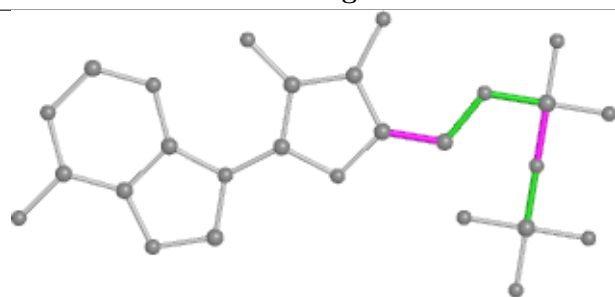
## Ligand ADP D 601



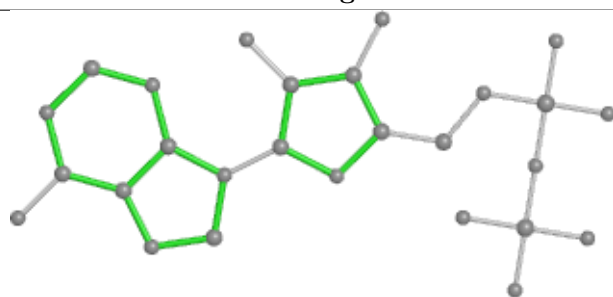
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

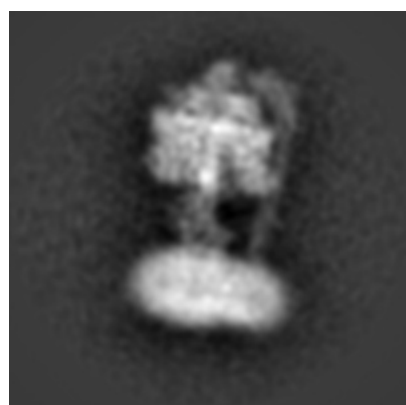
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8359. These allow visual inspection of the internal detail of the map and identification of artifacts.

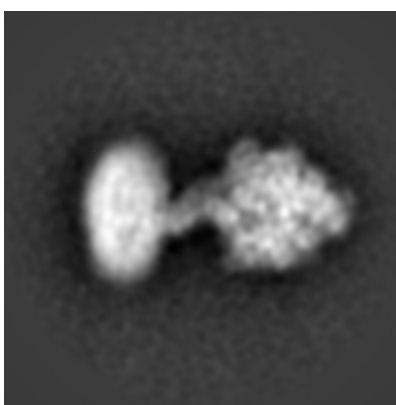
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

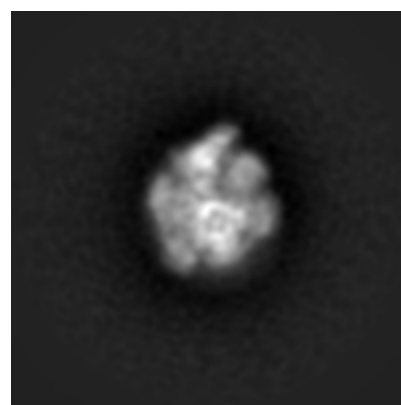
#### 6.1.1 Primary map



X



Y

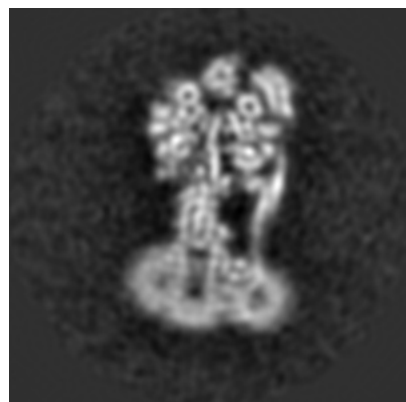


Z

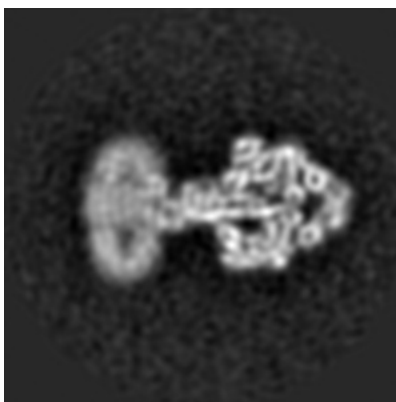
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

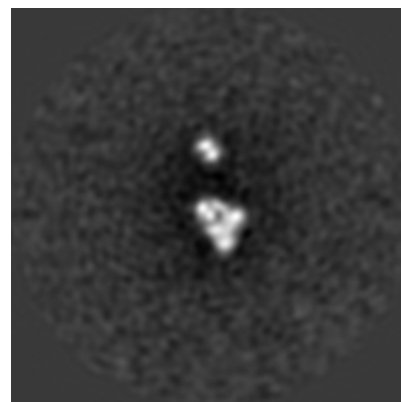
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

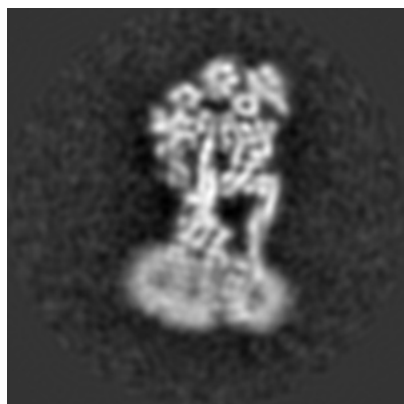


Z Index: 125

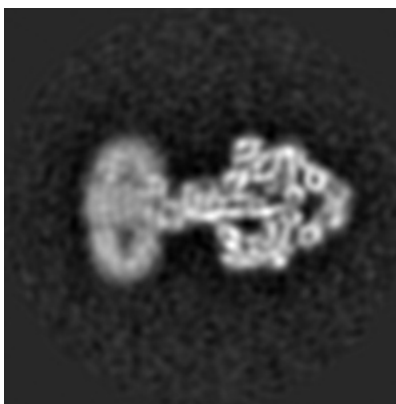
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

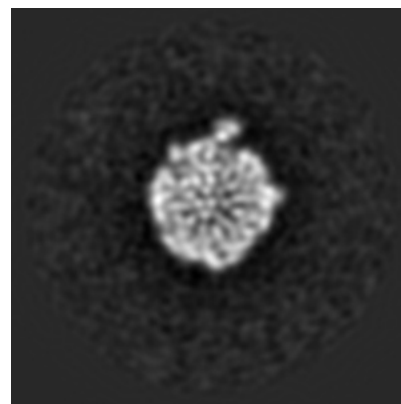
### 6.3.1 Primary map



X Index: 121



Y Index: 125

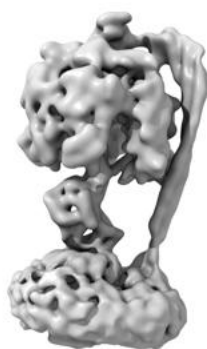


Z Index: 174

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

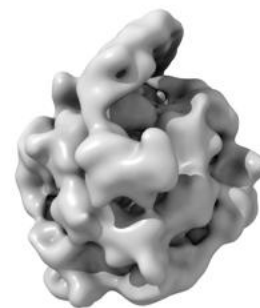
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

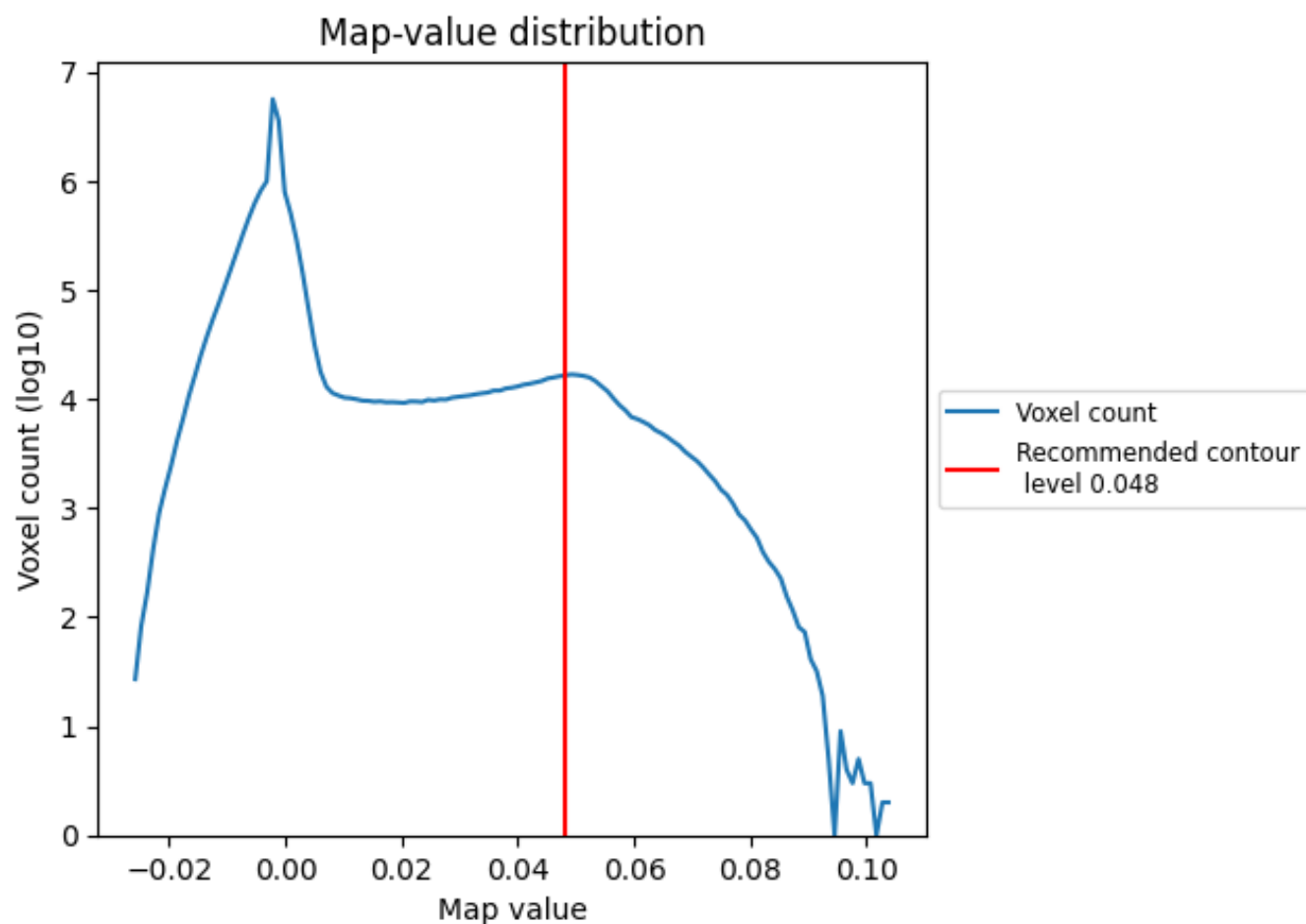
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

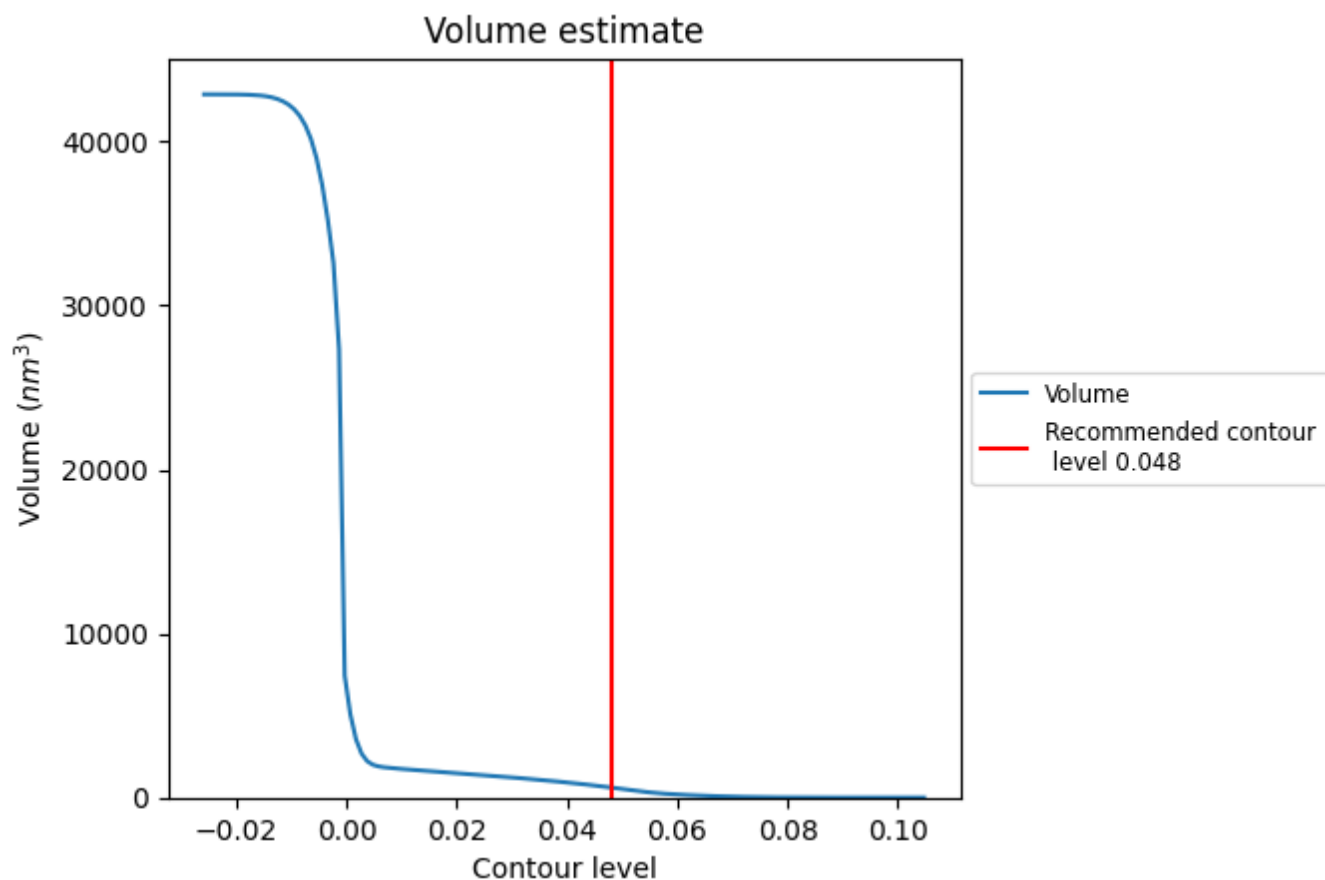
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

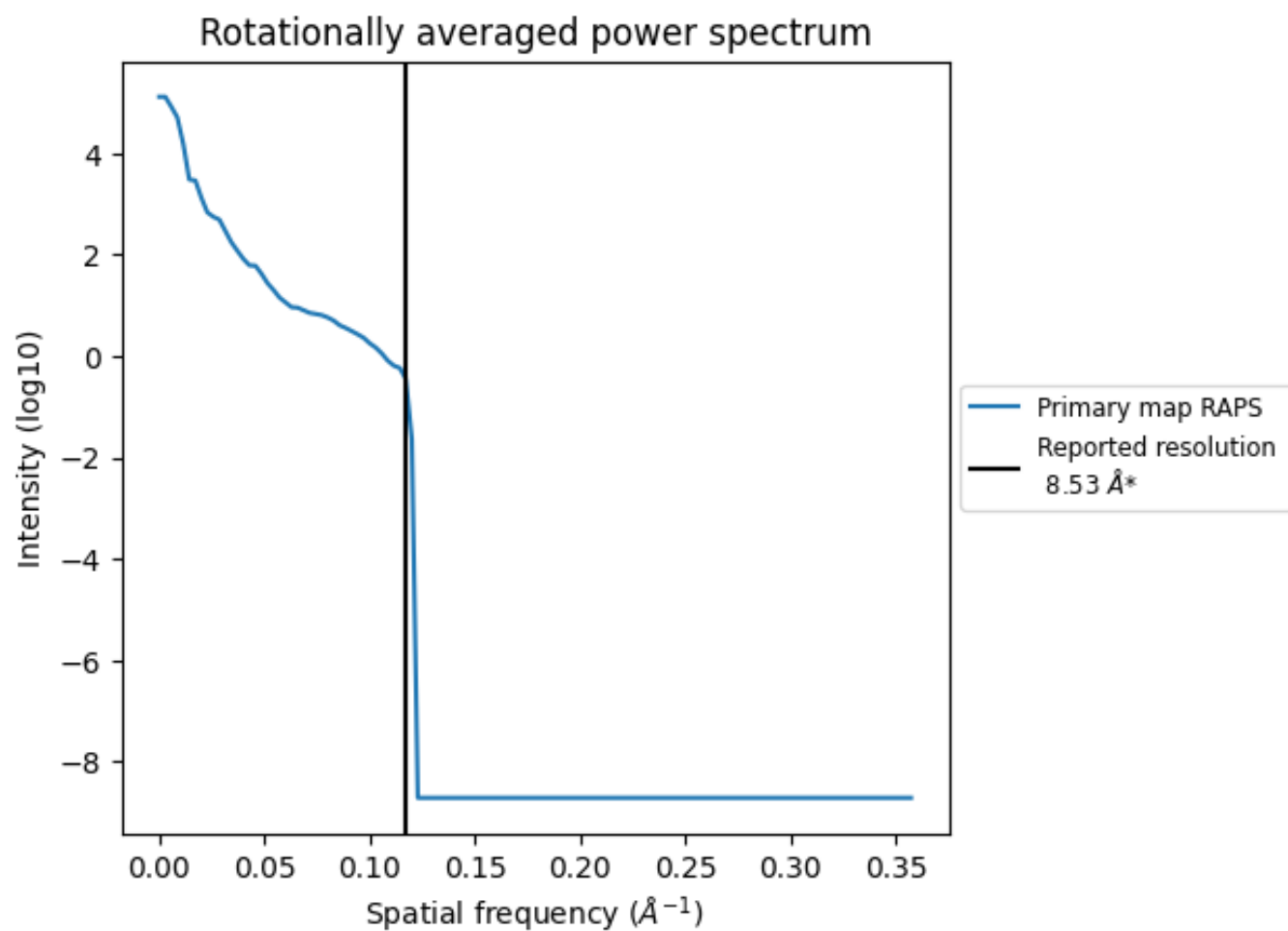


The volume at the recommended contour level is 612 nm<sup>3</sup>; this corresponds to an approximate mass of 553 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

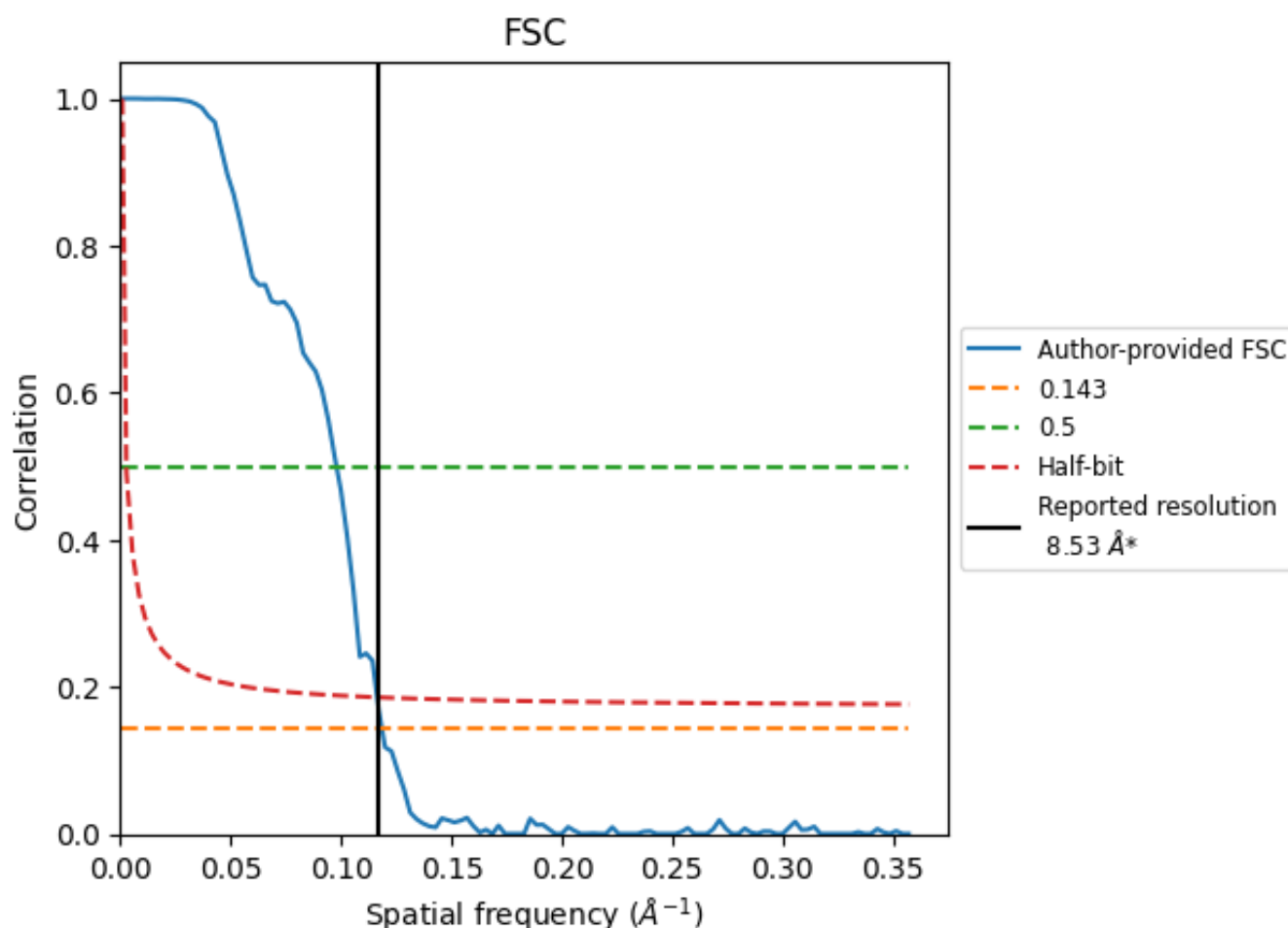


\*Reported resolution corresponds to spatial frequency of 0.117 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.117  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

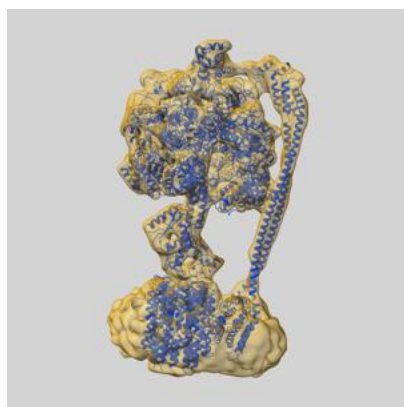
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.53	-	-
Author-provided FSC curve	8.43	10.20	8.59
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

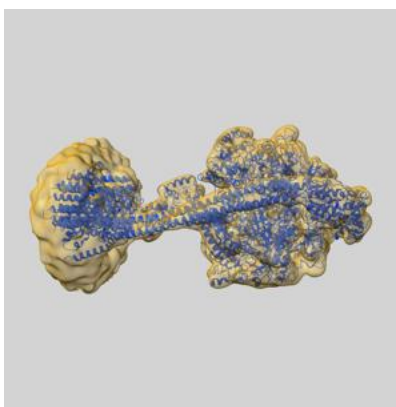
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8359 and PDB model 5T4Q. Per-residue inclusion information can be found in section [3](#) on page [10](#).

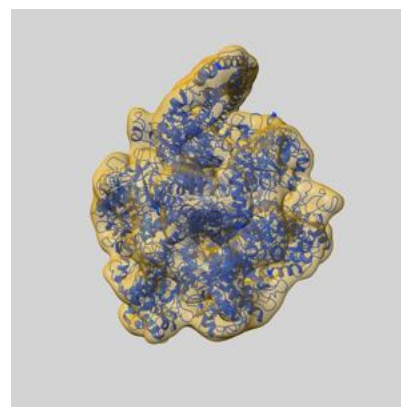
### 9.1 Map-model overlay [i](#)



X



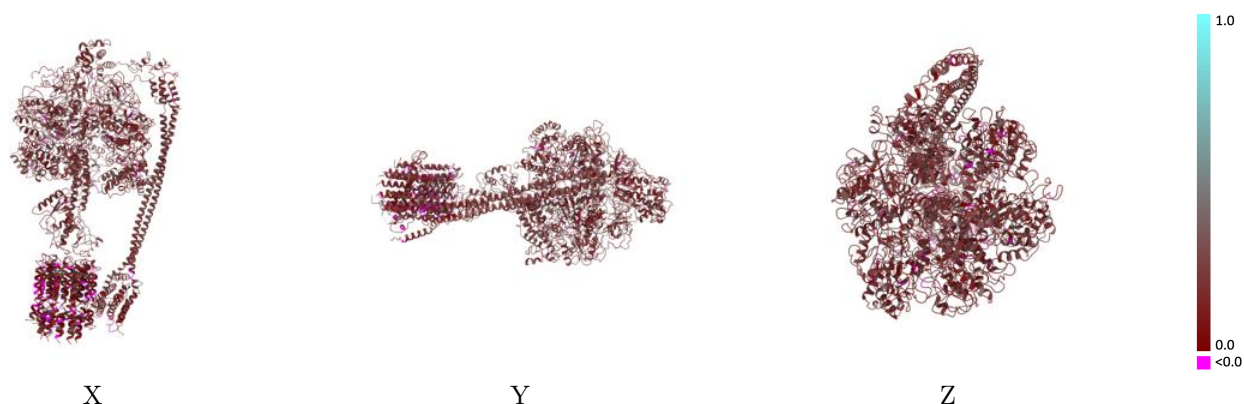
Y



Z

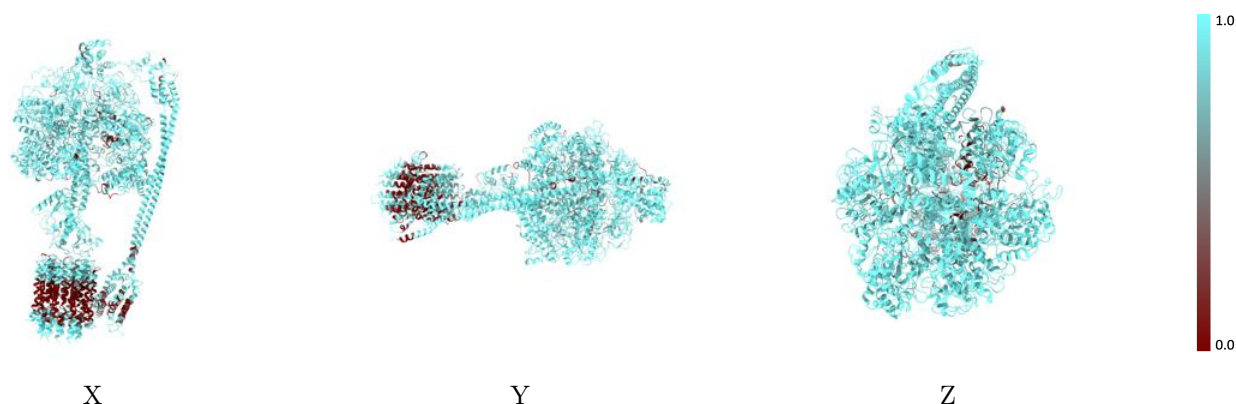
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



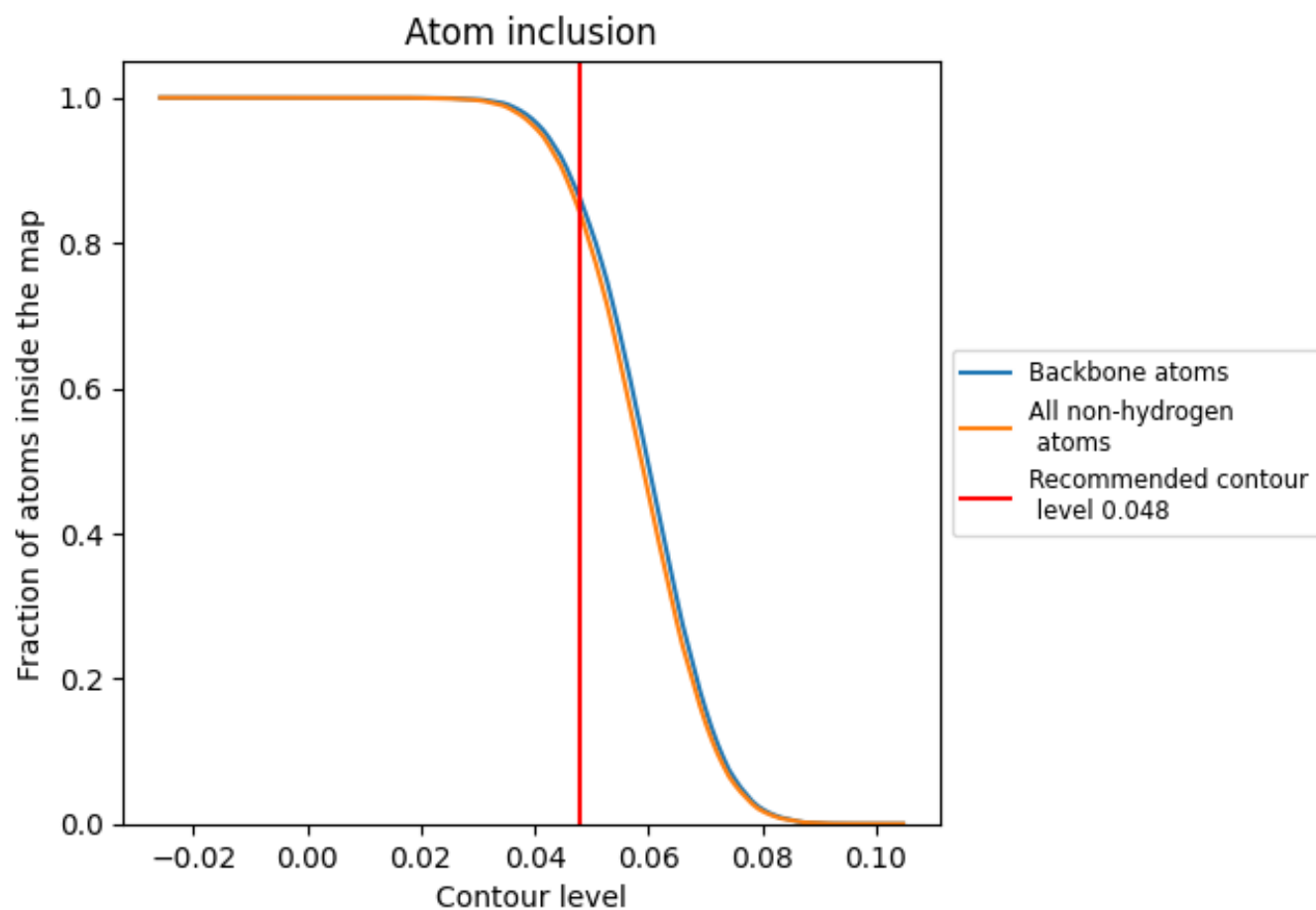
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.048).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8413	 0.1930
A	 0.9314	 0.2070
B	 0.9376	 0.2140
C	 0.9398	 0.2030
D	 0.9347	 0.2040
E	 0.8183	 0.1860
F	 0.9343	 0.2070
G	 0.9300	 0.2200
H	 0.8548	 0.2100
I	 0.8731	 0.2070
J	 0.8769	 0.2290
K	 0.6548	 0.1890
L	 0.9596	 0.2190
M	 0.5014	 0.0940
N	 0.5781	 0.1320
O	 0.4301	 0.1140
P	 0.4959	 0.1340
Q	 0.4822	 0.1470
R	 0.5589	 0.1570
S	 0.5096	 0.1100
T	 0.5616	 0.1330
U	 0.5205	 0.1190
V	 0.5370	 0.1070

